SPECTRUM OF ENGINEERING SCIENCES
ISSN (E) 3007-3138 (P) 3007-312X VOLUME 2, ISSUE 3, 2024

ANALYTICAL AND NUMERICAL INVESTIGATION OF MOSTAR, PI, AND SZEGED INDICES IN CARBON NANOTUBE STRUCTURE

Farhana Yasmeen[*1], Shehnaz Akhter[2], Mehtab Khan[3], Muhammad Uzair Khan[4], Aneesa Begum[5]

[*1]*Department of Mathematics, University of Okara, Okara, Pakistan*
[2]*School of Natural Sciences, National University of Sciences and Technology, Islamabad, Pakistan*
[3]*Department of Computer Science, Pakistan Global Institute, Rawalpindi, Pakistan*
[*4]*Department of Mathematics, University of Buner, Pakistan*
[5] *Government higher secondary school Rajjar,Charsad, KP Pakista*

[*1]shehnazakhter36@yahoo.com, [2]sumaira.hafeez@aack.au.edu.pk [3]mehtabkhan85@gmail.com, [4]uzairqau@gmail.com, [5]aneeszeb82@gmail.com

DOI: https://doi.org10.5281/zenodo.23364182

Keywords

Article History
Received: 01 January 2024
Accepted: 16 March 2024
Published: 31 March 2024

Copyright @Author
Corresponding Author: *
Muhammad Uzair Khan

Abstract

Topological indices are widely used in quantitative structure-activity and structure-property relationship studies in mathematical chemistry and are essential for describing the structural characteristics of chemical compounds. In this work, we examine the Mostar, Padmakar-Ivan (PI), and Szeged indices for carbon nanotube molecular graphs. We obtain precise closed-form expressions for vertex-distance, edge-distance, and total-distance based versions of these indices, including their weighted variants, by using the cut method. Additionally, a comparative numerical analysis is presented for various parameter values, showing that the Szeged indices follow a higher-order (hexic) growth pattern while the Mostar and PI indices show quadratic growth behavior. A clear visualization of the variation of these indices is provided by the tables and graphical representations of the computed results. The results emphasize the importance of topological descriptors in chemical graph theory and advance our knowledge of the structural properties of nanotube networks.

INTRODUCTION

The use of mathematical tools to model and analyze chemical structures is the main focus of mathematical chemistry, a significant area of theoretical chemistry. Graph theory, in particular, offers an effective framework for depicting molecular structures, treating chemical bonds as edges and atoms as vertices [5]. Through QSAR and QSPR studies, topological indices numerical parameters derived from such graphs are frequently used to predict the physicochemical characteristics and biological activities of chemical compounds [13, 14]. Due to their strong correlation with molecular structure and properties, distance-based indices have garnered a lot of attention among the different classes of topological indices. The Szeged index, the Padmakar-Ivan (PI) index, and the Mostar index are notable examples. Chemical graph theory and network analysis have made extensive use of the Szeged index, which was first introduced as an extension of the Wiener index. Khadikar [23] and associates developed the PI index, which offers important information about structural characteristics and molecular branching. A number of new developments and generalizations have resulted from the introduction of the Mostar

index as a measure of irregularity and peripherality in graphs in more recent times [20, 21, 22].

Let $H = (V_H, E_H)$ be a graph with the vertex set V_H and the edge set E_H, where $|V_H|$ and $|E_H|$ represents the order and size of H, respectively. The bond-additive topological invariants are largely employed to recognize the characteristics of chemical graphs. The Wiener invariant [28] is a first notable bond-additive invariant. Inspired by the miscellaneous productive invariants, such as Zagreb [10], irregularity [1], Szeged [11], and revised-Szeged [19, 24, 25]. Padmakar-Ivan a bond additive invariant PI was proposed by Khadikar et al [23]. For an edge $e = rz \in E_H$, there are two kinds of weights regarding degrees of end vertices.

$$W^*(e = rs) = deg_H(r)deg_H(s), W^+(e = rs) = deg_H(r) + deg_H(s).$$

Now, by using the above edge weights we can interpret the weighted PI invariants for H as:

$$\begin{aligned} W^+PI_v(H) &= \sum_{e=rs\in E_H} W^+(e=rs)(\mathrm{n}_r(e|H)+\mathrm{n}_s(e|H)),\\ W^+PI_e(H) &= \sum_{e=rs\in E_H} W^+(e=rs)(\mathrm{m}_r(e|H)+\mathrm{m}_s(e|H)),\\ W^+PI_t(H) &= \sum_{e=rs\in E_H} W^+(e=rs)(\mathrm{t}_r(e|H)+\mathrm{t}_s(e|H)),\\ W^*PI_v(H) &= \sum_{e=rs\in E_H} W^*(e=rs)(\mathrm{n}_r(e|H)+\mathrm{n}_s(e|H)),\\ W^*PI_e(H) &= \sum_{e=rs\in E_H} W^*(e=rs)(\mathrm{m}_r(e|H)+\mathrm{m}_s(e|H)),\\ W^*PI_t(H) &= \sum_{e=rs\in E_H} W^*(e=rs)(\mathrm{t}_r(e|H)+\mathrm{t}_s(e|H)). \end{aligned} \quad (1)$$

where $\mathrm{n}_r(e|H)$ (or $\mathrm{n}_s(e|H)$) is the cardinality of vertices closer to r (or s) than s (or r), $\mathrm{m}_r(e|H)$ (or $\mathrm{m}_s(e|H)$) is the cardinality of edges closer to r (or s) than s (or r), and $\mathrm{t}_r(e|H)$ (or $\mathrm{t}_s(e|H)$) is the cardinality of vertices and edges closer to r (or s) than s (or r). Farahani computed a closed formula for $PI_e(H)$ and $PI_v(H)$ of the structure of the circumcoronene series of benzenoid H_k by the use of cut method [9]. Farahani et al [8] computed the vertex PI index of Titania carbon Nanotubes $TiO_2[m,n]$. Zheng et al [29] computed the edge PI index of Titania carbon Nanotubes $TiO_2[m,n]$. In 1994, Gutman introduced Szeged Index [12] for any connected graph H by

$$Sz_v(H) = \sum_{rs\in E(H)} \mathrm{n}_r(e|H)\mathrm{n}_s(e|H) \qquad Sz_e(H) = \sum_{rs\in E(H)} \mathrm{m}_r(e|H)\mathrm{m}_s(e|H)$$
$$Sz_t(H) = \sum_{rs\in E(H)} \mathrm{t}_r(e|H)\mathrm{t}_s(e|H) \quad (2)$$

Now, by using the above edge weights we can interpret the weighted Szeged invariants for H as:

$$\begin{aligned} W^+Sz_v(H) &= \sum_{e=rs\in E_H} W^+(e=rs)\mathrm{n}_r(e|H)\mathrm{n}_s(e|H),\\ W^+Sz_e(H) &= \sum_{e=rs\in E_H} W^+(e=rs)\mathrm{m}_r(e|H)\mathrm{m}_s(e|H),\\ W^+Sz_t(H) &= \sum_{e=rs\in E_H} W^+(e=rs)\mathrm{t}_r(e|H)\mathrm{t}_s(e|H),\\ W^*Sz_v(H) &= \sum_{e=rs\in E_H} W^*(e=rs)\mathrm{n}_r(e|H)\mathrm{n}_s(e|H),\\ W^*Sz_e(H) &= \sum_{e=rs\in E_H} W^*(e=rs)\mathrm{m}_r(e|H)\mathrm{m}_s(e|H),\\ W^*Sz_t(H) &= \sum_{e=rs\in E_H} W^*(e=rs)\mathrm{t}_r(e|H)\mathrm{t}_s(e|H). \end{aligned} \quad (3)$$

The Szeged index has various critical applications in network theory and chemistry. Due to importance of Szeged index, several variations of this index including edge-Szeged index and the PI index were defined. In 2017, Doslić et al. [6] introduced the Monster index to acquire the peripherality measure of any given molecular structure and it was defined as follows:

$$Mo_v(H) = \sum_{rs\in E(H)} |\mathrm{n}_r(e|H) - \mathrm{n}_s(e|H)|. \quad (4)$$

Deng et al. [7] determined the Mostar invariant of benzenoid system. Further they found its extremal

Mostar invariant for trees and unicyclic graphs. Later the expression for the Mostar invariant of bicyclic graphs was derived in [26]. Tratnik [27] proved that the Mostar invariant of the weighted graph can be deduced in the form of Mostar invariant of quotient graphs. Recently, other versions of Mostar invariant, named as edge Mostar and total Mostar invariants, were presented by Arockiaraj et al. [2]. For more results related to Mostar invariants, see [3, 4, 15, 16]. These invariants are reported for H as:

$$Mo_e(H) = \sum_{rs\in E(H)} |\mathrm{m}_r(e|H) - \mathrm{m}_s(e|H)| \quad Mo_t(H) = \sum_{rs\in E(H)} |\mathrm{t}_r(e|H) - \mathrm{t}_s(e|H)| \quad (5)$$

Now, by using the above edge weights we can interpret the weighted Mostar invariants for H as:

$$\begin{aligned} W^+Mo_v(H) &= \sum_{e=rs\in E_H} W^+(e=rs)|\mathrm{n}_r(e|H) - \mathrm{n}_s(e|H)|, \\ W^+Mo_e(H) &= \sum_{e=rs\in E_H} W^+(e=rs)|\mathrm{m}_r(e|H) - \mathrm{m}_s(e|H)|, \\ W^+Mo_t(H) &= \sum_{e=rs\in E_H} W^+(e=rs)|\mathrm{t}_r(e|H) - \mathrm{t}_s(e|H)|, \\ W^*Mo_v(H) &= \sum_{e=rs\in E_H} W^*(e=rs)|\mathrm{n}_r(e|H) - \mathrm{n}_s(e|H)|, \\ W^*Mo_e(H) &= \sum_{e=rs\in E_H} W^*(e=rs)|\mathrm{m}_r(e|H) - \mathrm{m}_s(e|H)|, \\ W^*Mo_t(H) &= \sum_{e=rs\in E_H} W^*(e=rs)|\mathrm{t}_r(e|H) - \mathrm{t}_s(e|H)|. \end{aligned} \quad (6)$$

In the late $1950s$, they employ the cut method proposed in [17], which they used to determine the Wiener index of graphs. This approach was extended for general graphs by establishing a connection between the graph's canonical metric representation and its Wiener index in [18]. For a graph H the edges $e = rs$ and $f = r's'$ of H represents the the Djokovic-Winkler Θ relation if $d_H(rr') + d_H(ss') \neq d_H(rs) + d_H(r's')$. It is important to revise the substantial preliminaries of the Cut method which is critical to our computations. For any connected graph H, the edges $h = pq$ and $e = rs$ are in Djokovic-Winkler relation , whenever $d_H(p,r) + d_H(q,s) \neq d_H(p,s) + d_H(q,r)$.

In materials science and nano-technology, carbon nanotubes and hexagonal boron nitride nanotubes are significant nanostructures with exceptional chemical and physical characteristics. They are good candidates for graph-theoretical studies because of their regular lattice structures. The computation of different Mostar, PI, and Szeged indices for these nanotube structures is the main focus of this work. We obtain precise analytical expressions for vertex-distance, edge-distance, and total-distance based indices, including their weighted versions, using the cut method. We also offer graphical comparisons and numerical calculations to examine how these indices behave at various parameter values. In addition to expanding on previous findings in the literature, this study offers more profound understanding of the structural characteristics of nanotube networks.

Carbon nanotube graph

In this section, we use the cut method to calculate the Mostar, PI, and Szeged-type invariants of the carbon nanotube graph. As shown in Figure 1, the carbon nanotube graph, represented by $\mathbb{CNT}$, is a straightforward, connected, planar graph. Two families of hexagonal rings (includes vertical rings and horizontal rings) make up the structural components of a carbon nanotube. The first family has $\boldsymbol{\mu}$ vertical rings for a fixed parameter $\boldsymbol{\mu}$, whereas the second family has $\boldsymbol{\mu - 1}$ horizontal rings. For all $\boldsymbol{\mu \geq 2}$, the $\boldsymbol{\mu \times \mu}$ rectangular portion of the carbon nanotube graph has $\boldsymbol{6\mu^2 + 3\mu - 2}$ edges and $\boldsymbol{4\mu^2 + 4\mu - 1}$ vertices. These expressions result from the rectangular section's boundary conditions and the hexagons' regular arrangement. We break down the graph into edge-cuts that naturally divide the nanotube structure along its repeating units in order to apply the cut method. Figure 1 shows all of the cuts of the carbon nanotube graph that we used to calculate the topological indices. Depending on the distribution of vertices on opposite sides of the cut, each cut contributes to

the Mostar, PI, and Szeged indices. Each cut represents a unique class of parallel edges in the underlying hexagonal lattice. The geometric structure of $\mathbb{CNT}$ and the configuration of its edge-cuts are depicted in Figure 1, which serve as the basis for the analysis that follows.

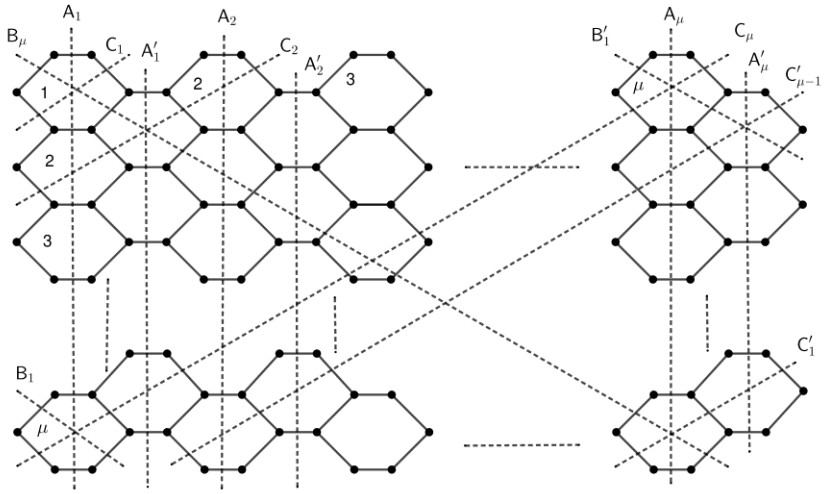


Figure 1: Carbon nanotube graph with edge cuts.

The cuts B_α and C_α, where $1 \le \alpha \le \mu$, are symmetric and $|B_\alpha| = |C_\alpha| = 2\alpha$

$$ccn_{B_\alpha}(z) = n_{C_\alpha}(z) = \alpha(2\alpha+1), n_{B_\alpha}(x) = n_{C_\alpha}(x) = 4\mu^2 + 4\mu - 1 - \alpha(2\alpha+1),$$
$$m_{B_\alpha}(z) = m_{C_\alpha}(z) = \alpha(3\alpha-1), m_{B_\alpha}(x) = m_{C_\alpha}(x) = 6\mu^2 + 3\mu - 2 - \alpha(3\alpha+1).$$

$$\left(d_{B_\alpha}(z), d_{B_\alpha}(x)\right) = \begin{cases} (2,3), & if\ 1 \le \alpha \le \mu\ and\ size\ is\ 2; \\ (3,3), & if\ 1 \le \alpha \le \mu\ and\ size\ is\ 2(\mu-1). \end{cases}$$
$$\left(d_{C_\alpha}(z), d_{C_\alpha}(x)\right) = \begin{cases} (2,3), & if\ 1 \le \alpha \le \mu-1\ and\ size\ is\ 2; \\ (3,3), & if\ 1 \le \alpha \le \mu\ and\ size\ is\ 2(\mu-1); \\ (2,2), & if\ \alpha = \mu\ and\ size\ is\ 2. \end{cases}$$

The cuts B'_α and C'_α, where $1 \le \alpha \le \mu - 1$, are symmetric and $|B'_\alpha| = |C'_\alpha| = 2\alpha + 1$

$$ccn_{B'_\alpha}(z) = n_{C'_\alpha}(z) = \alpha(2\alpha+3), n_{B'_\alpha}(x) = n_{C'_\alpha}(x) = 4\mu^2 + 4\mu - 1 - \alpha(2\alpha+3),$$
$$m_{B'_\alpha}(z) = m_{C'_\alpha}(z) = 3\alpha^2 + 2\alpha - 1, m_{B'_\alpha}(x) = m_{C'_\alpha}(x) = 6\mu^2 + 3\mu - 2 - (6\mu+1)\alpha.$$

$$\left(d_{C'_\alpha}(z), d_{C'_\alpha}(x)\right) = \begin{cases} (2,3), & if\ 1 \le \alpha \le \mu\ and\ size\ is\ 2; \\ (3,3), & if\ 1 \le \alpha \le \mu\ and\ size\ is\ 2\mu-1. \end{cases}$$
$$\left(d_{B'_\alpha}(z), d_{B'_\alpha}(x)\right) = \begin{cases} (2,3), & if\ 1 \le \alpha \le \mu-2\ and\ size\ is\ 2; \\ (3,3), & if\ 1 \le \alpha \le \mu-1\ and\ size\ is\ 2\mu-1; \\ (2,2), & if\ \alpha = \mu-1\ and\ size\ is\ 2. \end{cases}$$

For cuts A_α, where $1 \le \alpha \le \mu$, we have $|A_\alpha| = \mu + 1$ and

$$ccn_{A_\alpha}(z) = (2\mu+1)(2\alpha-1), n_{A_\alpha}(x) = 4\mu^2 + 2\mu - 2 - 2(2\mu-1)\alpha,$$
$$m_{A_\alpha}(z) = (6\mu+1)\alpha - (4\mu+1), m_{A_\alpha}(x) = 6\mu^2 + 6\mu - 2 - (6\mu+1)\alpha.$$

$$\left(d_{\mathrm{A}_\alpha}(z), d_{\mathrm{A}_\alpha}(x)\right) = \begin{cases}(2,2), & its\ size\ is\ 2;\\ (3,3), & its\ size\ is\ \mu-1.\end{cases}$$

For cuts $\mathrm{A'}_\alpha$, where $1 \le \alpha \le \mu$, we have $|\mathrm{A'}_\alpha| = \mu$, $d_{\mathcal{A}'_\alpha}(z) = d_{\mathcal{A}'_\alpha}(x) = 2$ and

$$ccn_{\mathrm{A}'_\alpha}(z) = 2(2\mu+1)\alpha, \mathrm{n}_{\mathrm{A}'_\alpha}(x) = 4\mu^2+4\mu-1-2(2\mu+1)\alpha,$$
$$\mathrm{m}_{\mathrm{A}'_\alpha}(z) = (6\mu+1)\alpha-\mu, \mathrm{m}_{\mathrm{A}'_\alpha}(x) = 6\mu^2+3\mu-2-(6\mu+1)\alpha.$$

We now calculate the carbon nanotube network's Mostar index and Szeged-type indices. The cut method mentioned above is used to perform these calculations, with each edge-cut contributing in accordance with the distribution of vertices on either side of the cut.

Theorem 2.1 *For $n \ge 2$, the Mostar indices for the network of hexagonal boron nitride are*

- $Mo_v(\mathbb{CNT}) = 8\mu^4 + \frac{32}{3}\mu^3 - 4\mu^2 - \frac{29}{3}\mu + 2 + (16\mu^3+16\mu^2-2)\left\lfloor\frac{\mu}{2}\right\rfloor - 4(2\mu+1)^2\left\lfloor\frac{\mu}{2}\right\rfloor^2.$
- $Mo_e(\mathbb{CNT}) = 12\mu^4 + 11\mu^3 - 10\mu^2 - 8\mu + 2 + (24\mu^3+18\mu^2-2\mu-4)\left\lfloor\frac{\mu}{2}\right\rfloor - 2(2\mu+1)(6\mu+1)\left\lfloor\frac{\mu}{2}\right\rfloor^2.$
- $Mo_t(\mathbb{CNT}) = 24\mu^4 + 22\mu^3 - 20\mu^2 - 16\mu + 4 + (40\mu^3+34\mu^2-2\mu-6)\left\lfloor\frac{\mu}{2}\right\rfloor - 2(2\mu+1)(10\mu+3)\left\lfloor\frac{\mu}{2}\right\rfloor^2.$

Proof. • By using the equation (4), we acquire

IEER
Institute for Excellence in Education & Research

$$Mo_v(\mathbb{CNT}) = 2\sum_{\alpha=1}^{\mu}(2\alpha)|4\mu^2+4\mu-1-\alpha(2\alpha+1)-\alpha(2\alpha+1)| + 2\sum_{\alpha=1}^{\mu-1}(2\alpha+1)|4\mu^2+4\mu$$
$$-1-\alpha(2\alpha+3)-\alpha(2\alpha+3)| + \sum_{\alpha=1}^{\mu}(\mu+1)|4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1)$$
$$-(2\mu+1)(2\alpha-1)| + \sum_{\alpha=1}^{\mu}\mu|4\mu^2+4\mu-1-2(2\mu+1)\alpha-2(2\mu+1)\alpha|$$
$$= 4(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu}(\alpha) - 8\sum_{i=1}^{\mu}(\alpha)^2(2\alpha+1) + 2(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu-1}(2\alpha+1)$$
$$-4\sum_{\alpha=1}^{\mu-1}\alpha(2\alpha+1)(2\alpha+3) + \sum_{\alpha=1}^{\lceil\frac{\mu}{2}\rceil}(\mu+1)(4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1)$$
$$-(2\mu+1)(2\alpha-1)) + \sum_{\lceil\frac{\mu}{2}\rceil+1}^{\mu}(\mu+1)((2\mu+1)(2\alpha-1)-(4\mu^2+4\mu-1$$
$$-(2\mu+1)(2\alpha-1))) + \sum_{\alpha=1}^{\lceil\frac{\mu}{2}\rceil}\mu(4\mu^2+4\mu-1-2(2\mu+1)\alpha-(2(2\mu+1)\alpha))$$
$$+\mu\sum_{\lceil\frac{\mu}{2}\rceil+1}^{\mu}(2(2\mu+1)\alpha-(4\mu^2+4\mu-1-2(2\mu+1)\alpha))$$
$$= 4(4\mu^2+4\mu-1)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right) - 8\left(\frac{1}{2}\mu^4+\frac{4}{3}\mu^3+\mu^2+\frac{1}{6}\mu\right) + 2(4\mu^2+4\mu$$
$$-1)(\mu^2-1) - 4\left(\mu^4+\frac{2}{3}\mu^3-\frac{3}{2}\mu^2-\frac{1}{6}\mu\right) + \left\lceil\frac{\mu}{2}\right\rceil(\mu+1)(-2(2\mu+1)$$

$$\left\lceil\frac{\mu}{2}\right\rceil + 4\mu^2+4\mu-1) + (\mu+1)\left(\mu-\left\lceil\frac{\mu}{2}\right\rceil\right)\left((4\mu+2)\left\lceil\frac{\mu}{2}\right\rceil-2\mu+1\right)$$
$$-\mu\left\lceil\frac{\mu}{2}\right\rceil(3-4\mu^2+(4\mu+2)\left\lceil\frac{\mu}{2}\right\rceil) + \mu\left(\mu-\left\lceil\frac{\mu}{2}\right\rceil\right)\left((4\mu+2)\left\lceil\frac{\mu}{2}\right\rceil+2\mu+3\right)$$
$$= 8\mu^4+\frac{32}{3}\mu^3-4\mu^2-\frac{29}{3}\mu+2+(16\mu^3+16\mu^2-2)\left\lceil\frac{\mu}{2}\right\rceil-4(2\mu+1)^2\left\lceil\frac{\mu}{2}\right\rceil^2.$$

- By using the equation (5), we acquire

$$Mo_e(\mathbb{CNT}) = 2\sum_{\alpha=1}^{\mu}(2\alpha)|6\mu^2+3\mu-2-\alpha(3\alpha+1)-\alpha(3\alpha-1)| + 2\sum_{\alpha=1}^{\mu-1}(2\alpha+1)|6\mu^2+3\mu$$

$$-2-3\alpha^2-4\alpha-(3\alpha^2+2\alpha-1)\Big|+\sum_{\alpha=1}^{\mu}(\mu+1)\Big|6\mu^2+6\mu-2-(6\mu+1)\alpha$$

$$-(6\mu+1)\alpha+(4\mu+1)|+\sum_{\alpha=1}^{\mu}\mu|6\mu^2+4\mu-2-(6\mu+1)\alpha-(6\mu+1)\alpha+\mu|$$

$$= 4(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}(\alpha) - 24\sum_{\alpha=1}^{\mu}(\alpha)^3 + 2(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu-1}(2\alpha+1)$$

$$-2\sum_{\alpha=1}^{\mu-1}(2\alpha+1)(6\alpha^2+6\alpha-1)+\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}(\mu+1)(6\mu^2+6\mu-2-(6\mu+1)\alpha$$

$$-(6\mu+1)\alpha+(4\mu+1))+\sum_{\left\lceil\frac{\mu}{2}\right\rceil+1}^{\mu}(\mu+1)((6\mu+1)\alpha-4\mu-1-6\mu^2$$

$$-6\mu+2+(6\mu+1)\alpha)+\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}\mu(6\mu^2+4\mu-2-(6\mu+1)\alpha-(6\mu+1)\alpha+\mu)$$

$$+\sum_{\left\lceil\frac{\mu}{2}\right\rceil+1}^{\mu}\mu\big((6\mu+1)\alpha-\mu-6\mu^2-4\mu+2+(6\mu+1)\alpha\big)$$

$$= 4(6\mu^2+3\mu-2)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right)-24\times\frac{1}{4}\mu^2(\mu+1)^2+2(6\mu^2+3\mu-2)(\mu^2-1)$$

$$-2(3\mu^4-4\mu^2+1)+\left\lceil\frac{\mu}{2}\right\rceil(\mu+1)\left(6\mu^2+4\mu-2-(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil\right)+(\mu+1)(\mu$$

$$-\left\lceil\frac{\mu}{2}\right\rceil)\left((6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil-3\mu+2\right)+\left\lceil\frac{\mu}{2}\right\rceil\mu(6\mu^2-\mu-3-(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil)$$

$$+\mu\left(\mu-\left\lceil\frac{\mu}{2}\right\rceil\right)\left((6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil+2\mu+3\right)$$

$$= 12\mu^4+11\mu^3-10\mu^2-8\mu+2+\qquad (24\mu^3+18\mu^2-2\mu-4)\left\lceil\frac{\mu}{2}\right\rceil$$

$$-2(2\mu+1)(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil^2.$$

[3.] By adding the values of $Mo_v(\mathbb{CNT})$ and $Mo_e(\mathbb{CNT})$, we get

$$Mo_t(\mathbb{CNT}) = 24\mu^4 + 22\mu^3 - 20\mu^2 - 16\mu + 4 + (40\mu^3 + 34\mu^2 - 2\mu - 6)\left\lceil\frac{\mu}{2}\right\rceil - 2(2\mu + 1)(10\mu + 3)\left\lceil\frac{\mu}{2}\right\rceil^2.$$

Theorem 2.2 *For $\mu \geq 2$, the Szeged indices for the network of hexagonal boron nitride are*

- $Sz_v(\mathbb{CNT}) = 16\mu^6 + \frac{664}{15}\mu^5 + 28\mu^4 - \frac{14}{3}\mu^3 - 5\mu^2 - \frac{3}{5}\mu.$
- $Sz_e(\mathbb{CNT}) = 36\mu^6 + 36\mu^5 - \frac{74}{3}\mu^4 - \frac{55}{2}\mu^3 + \frac{73}{6}\mu^2 + 8\mu - 4.$
- $Sz_t(\mathbb{CNT}) = 52\mu^6 + \frac{1204}{15}\mu^5 + \frac{10}{3}\mu^4 - \frac{193}{6}\mu^3 + \frac{43}{6}\mu^2 + \frac{37}{5}\mu - 4.$

Proof. • By using the equations (2), we acquire

IEER
Institute for Excellence in Education & Research

$$
\begin{aligned}
Sz_v(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu} 2\alpha(4\mu^2+4\mu-1-\alpha(2\alpha+1)(\alpha(2\alpha+1))+2\sum_{\alpha=1}^{\mu-1}(2\alpha+1)(4\mu^2+4\mu-1 \\
& -\alpha(2\alpha+3)(\alpha(2\alpha+3))+\sum_{\alpha=1}^{\mu}(\mu+1)(4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1)) \\
& ((2\mu+1)(2\alpha-1))+\sum_{\alpha=1}^{\mu}\mu(4\mu^2+4\mu-1-2(2\mu+1)\alpha)(2(2\mu+1)\alpha)) \\
= \; & 4(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu}\alpha^2(2\alpha+1)-4\sum_{\alpha=1}^{\mu}\alpha^3(2\alpha+1)^2+2(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu-1} \\
& \alpha(2\alpha+1)(2\alpha+3)-2\sum_{\alpha=1}^{\mu-1}\alpha^2(2\alpha+1)(2\alpha+3)^2+(4\mu^2+4\mu-1)(2\mu+1)(\mu+1) \\
& \sum_{\alpha=1}^{\mu}(2\alpha-1)-(2\mu+1)^2(\mu+1)\sum_{\alpha=1}^{\mu}(2\alpha-1)^2+2\mu(4\mu^2+4\mu-1)(2\mu+1)\sum_{\alpha=1}^{\mu}\alpha \\
& -4\mu(2\mu+1)^2\sum_{\alpha=1}^{\mu}\alpha^2 \\
= \; & 4(4\mu^2+4\mu-1)\left(\frac{1}{2}\mu^4+\frac{4}{3}\mu^3+\mu^2+\frac{1}{6}\mu\right)-4(\frac{2}{3}\mu^6+\frac{14}{5}\mu^5+\frac{47}{12}\mu^4+\frac{11}{6}\mu^3 \\
& -\frac{1}{12}\mu^2-\frac{2}{15}\mu)+2(4\mu^2+4\mu-1)\left(\mu^4+\frac{2}{3}\mu^3-\frac{3}{2}\mu^2-\frac{1}{6}\mu\right)-2(\frac{4}{3}\mu^6+\frac{8}{5}\mu^5 \\
& -\frac{19}{6}\mu^4-\frac{8}{3}\mu^3+\frac{7}{3}\mu^2+\frac{17}{30}\mu)+\mu^2(4\mu^2+4\mu-1)(2\mu+1)(\mu+1)-(2\mu+1)^2 \\
& (\mu+1)(\frac{4}{3}\mu^3-\frac{1}{3}\mu)+2\mu(4\mu^2+4\mu-1)(2\mu+1)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right) \\
& -4\mu(2\mu+1)^2\left(\frac{1}{3}\mu^3+\frac{1}{2}\mu^2+\frac{1}{6}\mu\right) \\
& = 16\mu^6+\frac{664}{15}\mu^5+28\mu^4-\frac{14}{3}\mu^3-5\mu^2-\frac{3}{5}\mu.
\end{aligned}
$$

[2.] By using the equations (2), we acquire

$$
\begin{aligned}
Sz_e(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu}(2\alpha)(6\mu^2+3\mu-2-\alpha(3\alpha+1))(\alpha(3\alpha-1))+2\sum_{\alpha=1}^{\mu-1}(2\alpha+1)(6\mu^2+3\mu-2 \\
& -\alpha(3\alpha+4))((3\alpha^2+2\alpha-1))+\sum_{\alpha=1}^{\mu}(\mu+1)(6\mu^2+6\mu-2-(6\mu+1)\alpha))((6\mu+1)\alpha \\
& -(4\mu+1))+\sum_{\alpha=1}^{\mu}\mu(6\mu^2+3\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-\mu) \\
= \; & 4(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}\alpha^2(3\alpha-1)-4\sum_{\alpha=1}^{\mu}\alpha^3(9\alpha^2-1)+2(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu-1}(2\alpha+1) \\
& (3\alpha^2+2\alpha-1)-2\sum_{\alpha=1}^{\mu-1}\alpha(2\alpha+1)(3\alpha+4)(3\alpha^2+2\alpha-1)+(6\mu^2+6\mu-2)(6\mu+1) \\
& (\mu+1)\sum_{\alpha=1}^{\mu}\alpha+(6\mu+1)(4\mu+1)(\mu+1)\sum_{\alpha=1}^{\mu}\alpha-(6\mu+1)^2(\mu+1)\sum_{\alpha=1}^{\mu}\alpha^2 \\
& -(6\mu^2+6\mu-2)(4\mu+1)(\mu+1)\sum_{\alpha=1}^{\mu}(1)+\mu(6\mu^2+3\mu-2)(6\mu+1)\sum_{\alpha=1}^{\mu}(\alpha) \\
& -\mu(6\mu+1)^2\sum_{\alpha=1}^{\mu}(\alpha)^2+\mu^2(6\mu+1)\sum_{\alpha=1}^{\mu}\alpha-\mu^2(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}(1) \\
= \; & 4(6\mu^2+3\mu-2)\left(\frac{3}{4}\mu^4+\frac{7}{6}\mu^3+\frac{1}{4}\mu^2-\frac{1}{6}\mu\right)-4(\frac{3}{2}\mu^6+\frac{9}{2}\mu^5+\frac{7}{2}\mu^4 \\
& -\frac{1}{2}\mu^3-\mu^2)+2(6\mu^2+3\mu-2)(\frac{3}{2}\mu^4-\frac{2}{3}\mu^3-2\mu^2+\frac{1}{6}\mu+1) \\
& -2(3\mu^6-8\mu^4+5\mu^2)+(6\mu^2+6\mu-2)(6\mu+1)(\mu+1)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right) \\
& +(6\mu+1)(4\mu+1)(\mu+1)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right)-(6\mu+1)^2(\mu+1)(\frac{1}{3}\mu^3+\frac{1}{2}\mu^2 \\
& +\frac{1}{6}\mu)-\mu(6\mu^2+6\mu-2)(4\mu+1)(\mu+1)+\mu(6\mu^2+3\mu-2)(6\mu+1)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right) \\
& -\mu(6\mu+1)^2\left(\frac{1}{3}\mu^3+\frac{1}{2}\mu^2+\frac{1}{6}\mu\right)+\mu^2(6\mu+1)\left(\frac{1}{2}\mu^2+\frac{1}{2}\mu\right)-\mu^3(6\mu^2+3\mu-2) \\
& = 36\mu^6+36\mu^5-\frac{74}{3}\mu^4-\frac{55}{2}\mu^3+\frac{73}{6}\mu^2+8\mu-4.
\end{aligned}
$$

[3.] By adding the values of $Sz_v(\mathbb{CNT})$ and $Sz_e(\mathbb{CNT})$, we get

$$Sz_t(\mathbb{CNT}) = 44\mu^6+\frac{324}{5}\mu^5-\frac{20}{3}\mu^4-\frac{169}{6}\mu^3+\frac{41}{3}\mu^2+\frac{161}{30}\mu-4.$$

The Mostar index, the weighted plus PI index, the weighted multiply PI index, the weighted plus Szeged index, the weighted multiply Szeged index, the weighted plus Mostar index, and the weighted multiply Mostar index are among the degree-distance based invariants of the carbon

nanotube network for which we derive explicit expressions in the analysis that follows. The cut method is used to calculate them; each fundamental edge-cut contributes to the corresponding index based on the sizes and degrees of the vertex partitions that the cut determines.

Theorem 2.3 *For $\mu \geq 2$, the weighted plus PI indices of hexagonal boron nitride are*

- $w^{+}PI_{v}(\mathbb{CNT}) = 144\mu^4 + 168\mu^3 - 60\mu^2 - 54\mu + 12.$
- $w^{+}PI_{e}(\mathbb{CNT}) = 216\mu^4 + 144\mu^3 - 54\mu^2 - 48\mu + 24.$
- $w^{+}PI_{t}(\mathbb{CNT}) = 360\mu^4 + 312\mu^3 - 114\mu^2 - 102\mu + 36.$

Proof. • Now, using the equations (1), we have

$$\begin{aligned}
w^{+}PI_{v}(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2+3)+2(3+3)(\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+1)+\alpha(2\alpha+1)) \\
& +(2(2+2)+2(3+3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1)+\mu(2\mu+1)) \\
& +(2(2+3)+2(3+3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1)+\mu(2\mu+1)) \\
& +2\sum_{\alpha=1}^{\mu-2}(2(2+3)+(3+3)(2\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+3)+\alpha(2\alpha+3)) \\
& +(2(2+3)+(3+3)(2(\mu-1)-1))(4\mu^2+4\mu-1-(\mu-1)(2(\mu-1)+3) \\
& +(\mu-1)(2(\mu-1)+3))+(2(2+2)+(3+3)(2(\mu-1)-1))(4\mu^2+4\mu-1 \\
& -(\mu-1)(2(\mu-1)+3)+(\mu-1)(2(\mu-1)+3))+\sum_{\alpha=1}^{\mu}(2(2+2)+(3+3) \\
& (\mu-1))(4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1)+(2\mu+1)(2\alpha-1)) \\
& +\sum_{\alpha=1}^{\mu}\mu(3+3)(4\mu^2+4\mu-1-2\alpha(2\mu+1)+2\alpha(2\mu+1)) \\
= \; & 4(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu-1}(6\alpha-1)+4(3\mu-1)(4\mu^2+4\mu-1)+2(6\mu-1)(4\mu^2 \\
& +4\mu-1)+8(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu-2}(3\alpha+1)+4(3\mu-2)(4\mu^2+4\mu-1)+2(6\mu \\
& -5)(4\mu^2+4\mu-1)+2(3\mu+1)(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu}(1)+6\mu(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu}(1) \\
= \; & 4(4\mu^2+4\mu-1)(3\mu^2-4\mu+1)+24(2\mu-1)(4\mu^2+4\mu-1)+4(4\mu^2+4\mu-1) \\
& (3\mu^2-7\mu+2)+2\mu(3\mu+1)(4\mu^2+4\mu-1)+6\mu^2(4\mu^2+4\mu-1) \\
& = 144\mu^4+168\mu^3-60\mu^2-54\mu+12.
\end{aligned}$$

- Now, using the equations (1), we have

$$
\begin{aligned}
w^{+}PI_e(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2+3)+2(3+3)(\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+1)+\alpha(3\alpha-1)) \\
& +(2(2+2)+2(3+3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1)+\mu(3\mu-1)) \\
& +(2(2+3)+2(3+3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1)+\mu(3\mu-1)) \\
& +2\sum_{\alpha=1}^{\mu-2}(2(2+3)+(3+3)(2\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+4)+(3\alpha^2+2\alpha \\
& -1))+(2(2+3)+(3+3)(2(\mu-1)-1))(6\mu^2+3\mu-2-(\mu-1)(3(\mu-1)+4) \\
& +(3(\mu-1)^2+2(\mu-1)-1))+(2(2+2)+(3+3)(2(\mu-1)-1))(6\mu^2+3\mu \\
& -2-(\mu-1)(3(\mu-1)+4)+(3(\mu-1)^2+2(\mu-1)-1))+\sum_{\alpha=1}^{\mu}(2(2+2) \\
& +(3+3)(\mu-1))(6\mu^2+6\mu-2-(6\mu+1)\alpha+((6\mu+1)\alpha-(4\mu+1))) \\
& +\sum_{\alpha=1}^{\mu}\mu(3+3)(6\mu^2+3\mu-2-(6\mu+1)\alpha+((6\mu+1)\alpha-\mu)) \\
= \; & 4(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu-1}(6\alpha-1)+4(3\mu-1)(6\mu^2+3\mu-2)+2(6\mu-1)(6\mu^2+3\mu \\
& -2)+8(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu-2}(3\alpha+1)+4(3\mu-2)(6\mu^2+3\mu-2)+2(6\mu-5) \\
& (6\mu^2+3\mu-2)+2(3\mu+1)(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}(1)+6\mu(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}(1) \\
= \; & 4(6\mu^2+3\mu-2)(3\mu^2-4\mu+1)+24(2\mu-1)(6\mu^2+3\mu-2)+4(6\mu^2+3\mu-2) \\
& (3\mu^2-7\mu+2)+2\mu(3\mu+1)(6\mu^2+3\mu-2)+6\mu^2(6\mu^2+3\mu-2) \\
& =216\mu^4+144\mu^3-54\mu^2-48\mu+24.
\end{aligned}
$$

- By adding the values of $w^{+}PI_v(\mathbb{CNT})$ and $w^{+}PI_e(\mathbb{CNT})$, we get

$$w^{+}PI_t(\mathbb{CNT}) = 360\mu^4+312\mu^3-114\mu^2-102\mu+36.$$

Theorem 2.4 *For $\mu \geq 2$, the weighted plus PI indices of hexagonal boron nitride are*

- $w^{*}PI_v(\mathbb{CNT}) = 216\mu^4+156\mu^3-98\mu^2+31\mu-4.$
- $w^{*}PI_e(\mathbb{CNT}) = 324\mu^4+72\mu^3-129\mu^2+42\mu-8.$
- $w^{*}PI_t(\mathbb{CNT}) = 540\mu^4+228\mu^3-227\mu^2+73\mu-12.$

Proof. • Now, using the equations (1), we have

$$
\begin{aligned}
w^*PI_v(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2\times 3)+2(3\times 3)(\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+1)+\alpha(2\alpha+1)) \\
& +(2(2\times 2)+2(3\times 3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1)+\mu(2\mu+1)) \\
& +(2(2\times 3)+2(3\times 3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1)+\mu(2\mu+1)) \\
& +2\sum_{\alpha=1}^{\mu-2}(2(2\times 3)+(3\times 3)(2\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+3)+\alpha(2\alpha+3)) \\
& +(2(2\times 3)+(3\times 3)(2(\mu-1)-1))(4\mu^2+4\mu-1-(\mu-1)(2(\mu-1)+3) \\
& +(\mu-1)(2(\mu-1)+3))+(2(2\times 2)+(3\times 3)(2(\mu-1)-1))(4\mu^2+4\mu-1 \\
& -(\mu-1)(2(\mu-1)+3)+(\mu-1)(2(\mu-1)+3))+\sum_{\alpha=1}^{\mu}(2(2\times 2)+(3\times 3) \\
& (\mu-1))(4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1)+(2\mu+1)(2\alpha-1)) \\
& +\sum_{\alpha=1}^{\mu}\mu(3\times 3)(4\mu^2+4\mu-1-2\alpha(2\mu+1)+2\alpha(2\mu+1)) \\
= \; & 12(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu-1}(3\alpha-1)+2(9\mu-5)(4\mu^2+4\mu-1)+6(3\mu-1)(4\mu^2 \\
& +4\mu-1)+6(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu-2}(6\alpha+1)+6(3\mu-1)(4\mu^2+4\mu-1)+2(9\mu-5) \\
& (4\mu^2+4\mu-1)+(9\mu-1)(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu}(1)+9\mu(4\mu^2+4\mu-1)\sum_{\alpha=1}^{\mu}(1) \\
= \; & 6(4\mu^2+4\mu-1)(3\mu^2-5\mu+2)+8(9\mu-4)(4\mu^2+4\mu-1)+6(4\mu^2+4\mu-1) \\
& (3\mu^2-8\mu+4)+\mu(9\mu-1)(4\mu^2+4\mu-1)+9\mu^2(4\mu^2+4\mu-1) \\
& =216\mu^4+156\mu^3-98\mu^2+31\mu-4.
\end{aligned}
$$

- Now, using the equations (1), we have

$$
\begin{aligned}
w^*PI_e(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2\times 3)+2(3\times 3)(\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+1)+\alpha(3\alpha-1)) \\
& +(2(2\times 2)+2(3\times 3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1)+\mu(3\mu-1)) \\
& +(2(2\times 3)+2(3\times 3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1)+\mu(3\mu-1)) \\
& +2\sum_{\alpha=1}^{\mu-2}(2(2\times 3)+(3\times 3)(2\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+4)+(3\alpha^2+2\alpha \\
& -1))+(2(2\times 3)+(3\times 3)(2(\mu-1)-1))(6\mu^2+3\mu-2-(\mu-1)(3(\mu-1)+4)
\end{aligned}
$$

$$+(3(\mu-1)^2+2(\mu-1)-1))+(2(2\times 2)+(3\times 3)(2(\mu-1)-1))(6\mu^2+3\mu$$
$$-2-(\mu-1)(3(\mu-1)+4)+(3(\mu-1)^2+2(\mu-1)-1))+\sum_{\alpha=1}^{\mu}(2(2\times 2)$$
$$+(3\times 3)(\mu-1))(6\mu^2+6\mu-2-(6\mu+1)\alpha+((6\mu+1)\alpha-(4\mu+1)))$$
$$+\sum_{\alpha=1}^{\mu}\mu(3\times 3)(6\mu^2+3\mu-2-(6\mu+1)\alpha+((6\mu+1)\alpha-\mu))$$

$$= 12(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu-1}(3\alpha-1)+2(9\mu-5)(6\mu^2+3\mu-2)+6(3\mu-1)(6\mu^2+3\mu$$
$$-2)+6(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu-2}(6\alpha+1)+6(3\mu-2)(6\mu^2+3\mu-2)+2(9\mu-5)$$
$$(6\mu^2+3\mu-2)+(9\mu-1)(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}(1)+9\mu(6\mu^2+3\mu-2)\sum_{\alpha=1}^{\mu}(1)$$
$$= 6(6\mu^2+3\mu-2)(3\mu^2-5\mu+2)+8(9\mu-4)(6\mu^2+3\mu-2)+6(6\mu^2+3\mu-2)$$
$$(3\mu^2-8\mu+4)+\mu(9\mu-1)(6\mu^2+3\mu-2)+9\mu^2(6\mu^2+3\mu-2)$$
$$= 324\mu^4+72\mu^3-129\mu^2+42\mu-8.$$

- By adding the values of $w^*PI_v(\mathbb{CNT})$ and $w^*PI_e(\mathbb{CNT})$, we get

$$w^*PI_t(\mathbb{CNT}) = 540\mu^4+228\mu^3-227\mu^2+73\mu-12.$$

IEER Institute for Excellence in Education & Research

Theorem 2.5 *For $\mu \geq 2$, the weighted plus Szeged indices of hexagonal boron nitride are*

- $w^+Sz_v(\mathbb{CNT}) = 96\mu^6+240\mu^5-8\mu^4-\frac{172}{3}\mu^3+126\mu^2-\frac{38}{3}\mu-36.$
- $w^+Sz_e(\mathbb{CNT}) = 180\mu^6+\frac{822}{5}\mu^5-94\mu^4-\frac{322}{3}\mu^3-127\mu^2+\frac{2279}{15}\mu-16.$
- $w^+Sz_t(\mathbb{CNT}) = 276\mu^6+\frac{2022}{5}\mu^5-102\mu^4-\frac{494}{3}\mu^3-\mu^2+\frac{2089}{15}\mu-52.$

Proof. • Now, using the equations (3), we have

$$w^+Sz_v(\mathbb{CNT}) = 2\sum_{\alpha=1}^{\mu-1}(2(2+3)+2(3+3)(\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+1))(\alpha(2\alpha+1))$$
$$+(2(2+2)+2(3+3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1))(\mu(2\mu+1))$$
$$+(2(2+3)+2(3+3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1))(\mu(2\mu+1))$$
$$+2\sum_{\alpha=1}^{\mu-2}(2(2+3)+(3+3)(2\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+3))(\alpha(2\alpha+3))$$

$$+(2(2+3)+(3+3)(2(\mu-1)-1))(4\mu^2+4\mu-1-(\mu-1)(2(\mu-1)+3))$$
$$((\mu-1)(2(\mu-1)+3))+(2(2+2)+(3+3)(2(\mu-1)-1))(4\mu^2+4\mu-1$$
$$-(\mu-1)(2(\mu-1)+3))((\mu-1)(2(\mu-1)+3))+\sum_{\alpha=1}^{\mu}(2(2+2)+(3+3)$$
$$(\mu-1))(4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1))((2\mu+1)(2\alpha-1))$$
$$+\sum_{\alpha=1}^{\mu}\mu(3+3)(4\mu^2+4\mu-1-2\alpha(2\mu+1))(2\alpha(2\mu+1))$$

$$= 4\sum_{\alpha=1}^{\mu-1}\alpha(6\alpha-1)(2\alpha+1)(4\mu^2+4\mu-1-\alpha(2\alpha+1))$$
$$+4\mu(2\mu+1)(3\mu-1)(2\mu^2+3\mu-1)+2\mu(2\mu+1)(6\mu-1)(2\mu^2+3\mu-1)$$
$$+8\sum_{\alpha=1}^{\mu-2}\alpha(2\alpha+3)(3\alpha+1)(4\mu^2+4\mu-1-\alpha(2\alpha+3))$$
$$+4(3\mu-2)(\mu-1)(2\mu+1)(2\mu^2+3\mu-2)+2(\mu-1)(2\mu+1)(6\mu-5)(2\mu^2+3\mu-2)$$
$$+4(3\mu+1)(2\mu+1)\sum_{\alpha=1}^{\mu}(2\alpha-1)(2\mu^2+3\mu-2\mu\alpha-\alpha)$$
$$+12\mu(2\mu+1)\sum_{\alpha=1}^{\mu}\alpha(4\mu^2+4\mu-1-4\alpha\mu-2\alpha)$$

$$= \frac{2}{3}\mu(\mu-1)(48\mu^4+56\mu^3-65\mu^2-29\mu+2)+6(2\mu+1)(16\mu^4+8\mu^3-30\mu^2+24\mu-6)$$
$$+\frac{2}{3}\mu(48\mu^5-64\mu^4-235\mu^3+370\mu^2+7\mu-126)+\frac{2}{3}\mu(3\mu+1)(2\mu+1)$$
$$(4\mu^3+8\mu^2-\mu+1)+2\mu^2(2\mu+1)(\mu+1)(4\mu^2+4\mu-5)$$
$$= 96\mu^6+240\mu^5-8\mu^4-\frac{172}{3}\mu^3+126\mu^2-\frac{38}{3}\mu-36.$$

- Now, using the equations (3), we have

$$w^+Sz_e(\mathbb{CNT}) = 2\sum_{\alpha=1}^{\mu-1}(2(2+3)+2(3+3)(\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+1))(\alpha(3\alpha-1))$$
$$+(2(2+2)+2(3+3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1))(\mu(3\mu-1))$$
$$+(2(2+3)+2(3+3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1))(\mu(3\mu-1))$$
$$+2\sum_{\alpha=1}^{\mu-2}(2(2+3)+(3+3)(2\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+4))((3\alpha^2+2\alpha$$
$$-1))+(2(2+3)+(3+3)(2(\mu-1)-1))(6\mu^2+3\mu-2-(\mu-1)(3(\mu-1)$$
$$+4))(3(\mu-1)^2+2(\mu-1)-1))+(2(2+2)+(3+3)(2(\mu-1)-1))(6\mu^2$$

$$
\begin{aligned}
&+3\mu-2-(\mu-1)(3(\mu-1)+4))((3(\mu-1)^2+2(\mu-1)-1))+\sum_{\alpha=1}^{\mu}(2(2+2)\\
&+(3+3)(\mu-1))(6\mu^2+6\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-(4\mu+1))\\
&+\sum_{\alpha=1}^{\mu}\mu(3+3)(6\mu^2+3\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-\mu)\\
=\;& 4\sum_{\alpha=1}^{\mu-1}\alpha(3\alpha-1)(6\alpha-1)(6\mu^2+3\mu-2-\alpha(3\alpha+1))\\
&+4\mu(3\mu-1)^2(3\mu^2+2\mu-2)+2\mu(3\mu-1)(6\mu-1)(3\mu^2+2\mu-2)\\
&+8\sum_{\alpha=1}^{\mu-2}(3\alpha+1)(3\alpha^2+2\alpha-1)(6\mu^2+3\mu-2-\alpha(3\alpha+4))\\
&+4(3\mu-2)(3\mu^2-4\mu)(3\mu^2+6\mu+1)+2(6\mu-5)(3\mu^2-4\mu)(3\mu^2+6\mu+1)\\
&+2(3\mu+1)\sum_{\alpha=1}^{\mu}(6\mu^2+6\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-(4\mu+1))\\
&+6\mu\sum_{\alpha=1}^{\mu}(6\mu^2+3\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-\mu)\\
=\;& \frac{2}{15}\mu(\mu-1)(540\mu^4-351\mu^3-756\mu^2+449\mu-106)+6\mu(72\mu^4-137\mu^2+63\mu+10)\\
&+72\mu^6-\frac{1134}{5}\mu^5-36\mu^4+\frac{1766}{3}\mu^3-408\mu^2+\frac{1232}{15}\mu-16+36\mu^6\\
&+42\mu^5-34\mu^4-\frac{26}{3}\mu^3+10\mu^2+\frac{8}{3}\mu+\mu(36\mu^4+30\mu^3-26\mu^2-33\mu-7)\\
&=180\mu^6+\frac{822}{5}\mu^5-94\mu^4-\frac{322}{3}\mu^3-127\mu^2+\frac{2279}{15}\mu-16.
\end{aligned}
$$

- By adding the values of $w^+Sz_v(\mathbb{CNT})$ and $w^+Sz_e(\mathbb{CNT})$, we get

$$w^+Sz_t(\mathbb{CNT})=276\mu^6+\tfrac{2022}{5}\mu^5-102\mu^4-\tfrac{494}{3}\mu^3-\mu^2+\tfrac{2089}{15}\mu-52.$$

Theorem 2.6 *For $\mu\geq 2$, the weighted multiply Szeged indices of hexagonal boron nitride are*

- $w^*Sz_v(\mathbb{CNT})=660\mu^6+\frac{3946}{15}\mu^5-\frac{4432}{3}\mu^4+\frac{1127}{2}\mu^3+\frac{1348}{3}\mu^2-\frac{2537}{30}\mu-32.$
- $w^*Sz_e(\mathbb{CNT})=288\mu^6+207\mu^5-8\mu^4-\frac{199}{6}\mu^3-\frac{1165}{2}\mu^2+\frac{632}{3}\mu-12.$
- $w^*Sz_t(\mathbb{CNT})=948\mu^6+\frac{7051}{15}\mu^5-\frac{4456}{3}\mu^4+\frac{1591}{3}\mu^3-\frac{799}{6}\mu^2+\frac{1261}{10}\mu-44.$

Proof. • Now, using the equations (3), we have

$$
\begin{aligned}
w^*Sz_v(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2\times 3)+2(3\times 3)(\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+1))(\alpha(2\alpha+1)) \\
& +(2(2\times 2)+2(3\times 3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1))(\mu(2\mu+1)) \\
& +(2(2\times 3)+2(3\times 3)(\mu-1))(4\mu^2+4\mu-1-\mu(2\mu+1))(\mu(2\mu+1)) \\
& +2\sum_{\alpha=1}^{\mu-2}(2(2\times 3)+(3\times 3)(2\alpha-1))(4\mu^2+4\mu-1-\alpha(2\alpha+3))(\alpha(2\alpha+3)) \\
& +(2(2\times 3)+(3\times 3)(2(\mu-1)-1))(4\mu^2+4\mu-1-(\mu-1)(2(\mu-1)+3)) \\
& ((\mu-1)(2(\mu-1)+3))+(2(2\times 2)+(3\times 3)(2(\mu-1)-1))(4\mu^2+4\mu-1 \\
& -(\mu-1)(2(\mu-1)+3))((\mu-1)(2(\mu-1)+3))+\sum_{\alpha=1}^{\mu}(2(2\times 2)+(3\times 3) \\
& (\mu-1))(4\mu^2+4\mu-1-(2\mu+1)(2\alpha-1))((2\mu+1)(2\alpha-1)) \\
& +\sum_{\alpha=1}^{\mu}\mu(3\times 3)(4\mu^2+4\mu-1-2\alpha(2\mu+1))(2\alpha(2\mu+1)) \\
= \; & 12\sum_{\alpha=1}^{\mu-1}\alpha(3\alpha-1)(2\alpha+1)(4\mu^2+4\mu-1-\alpha(2\alpha+1)) \\
& +2\mu(2\mu+1)(9\mu-5)(2\mu^2+3\mu-1)+6\mu(2\mu+1)(3\mu-1)(2\mu^2+3\mu-1) \\
& +6\sum_{\alpha=1}^{\mu-2}\alpha(2\alpha+3)(6\alpha+1)(4\mu^2+4\mu-1-\alpha(2\alpha+3)) \\
& +6(3\mu-1)(\mu-1)(2\mu+1)(2\mu^2+3\mu-2)+2(\mu-1)(2\mu+1)(9\mu-5) \\
& (2\mu^2+3\mu-2)+(9\mu-1)(2\mu+1)\sum_{\alpha=1}^{\mu}(2\alpha-1)(2\mu^2+3\mu-2\mu\alpha-\alpha) \\
& +18\mu(2\mu+1)\sum_{\alpha=1}^{\mu}\alpha(4\mu^2+4\mu-1-4\alpha\mu-2\alpha) \\
= \; & \frac{12}{5}\mu(\mu-1)(240\mu^4+224\mu^3-431\mu^2-161\mu+14)+288\mu^5+304\mu^4-480\mu^3 \\
& +56\mu^2+104\mu-32+48\mu^6-\frac{376}{5}\mu^5-233\mu^4+428\mu^3-13\mu^2-\frac{774}{5}\mu+\frac{1}{6}\mu \\
& (9\mu-1)(2\mu+1)(4\mu^3+8\mu^2-\mu+1)+3\mu^2(2\mu+1)(\mu+1)(4\mu^2+4\mu-5) \\
= \; & 660\mu^6+\frac{3946}{15}\mu^5-\frac{4432}{3}\mu^4+\frac{1127}{2}\mu^3+\frac{1348}{3}\mu^2-\frac{2537}{30}\mu-32.
\end{aligned}
$$

- Now, using the equations (3), we have

$$
\begin{aligned}
w^*Sz_e(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2\times 3)+2(3\times 3)(\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+1))(\alpha(3\alpha-1)) \\
& +(2(2\times 2)+2(3\times 3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1))(\mu(3\mu-1))
\end{aligned}
$$

$$
\begin{aligned}
&+(2(2\times 3)+2(3\times 3)(\mu-1))(6\mu^2+3\mu-2-\mu(3\mu+1))(\mu(3\mu-1))\\
&+2\sum_{\alpha=1}^{\mu-2}(2(2\times 3)+(3\times 3)(2\alpha-1))(6\mu^2+3\mu-2-\alpha(3\alpha+4))((3\alpha^2+2\alpha\\
&-1))+(2(2\times 3)+(3\times 3)(2(\mu-1)-1))(6\mu^2+3\mu-2-(\mu-1)(3(\mu-1)+4))\\
&((3(\mu-1)^2+2(\mu-1)-1))+(2(2\times 2)+(3\times 3)(2(\mu-1)-1))(6\mu^2+3\mu\\
&-2-(\mu-1)(3(\mu-1)+4))((3(\mu-1)^2+2(\mu-1)-1))+\sum_{\alpha=1}^{\mu}(2(2\times 2)\\
&+(3\times 3)(\mu-1))(6\mu^2+6\mu-2-(6\mu+1)\alpha)(((6\mu+1)\alpha-(4\mu+1)))\\
&+\sum_{\alpha=1}^{\mu}\mu(3\times 3)(6\mu^2+3\mu-2-(6\mu+1)\alpha)(((6\mu+1)\alpha-\mu))\\
=\;& 12\sum_{\alpha=1}^{\mu-1}\alpha(3\alpha-1)(2\alpha+1)(6\mu^2+3\mu-2-\alpha(3\alpha+1))\\
&+2\mu(2\mu+1)(9\mu-5)(3\mu^2+2\mu-2)+6\mu(3\mu-1)(2\mu+1)(3\mu^2+2\mu-2)\\
&+6\sum_{\alpha=1}^{\mu-2}(6\alpha+1)(3\alpha^2+2\alpha-1)(6\mu^2+3\mu-2-\alpha(3\alpha+4))\\
&+6(3\mu-1)(3\mu^2-4\mu)(3\mu^2+6\mu+1)+2(9\mu-5)(3\mu^2-4\mu)(3\mu^2+6\mu+1)\\
&+(9\mu-1)\sum_{\alpha=1}^{\mu}(6\mu^2+6\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-(4\mu+1))\\
&+9\mu\sum_{\alpha=1}^{\mu}(6\mu^2+3\mu-2-(6\mu+1)\alpha)((6\mu+1)\alpha-\mu)\\
=\;& 72\mu^6-\tfrac{258}{5}\mu^5-126\mu^4+86\mu^3+30\mu^2-\tfrac{52}{5}\mu+540\mu^5+228\mu^4-1036\mu^3+152\mu^2+96\mu\\
&+\tfrac{1}{5}(540\mu^6-1827\mu^5+4750\mu^3-3825\mu^2+632\mu-60)+(9\mu-1)(6\mu^5+5\mu^4-\tfrac{22}{3}\mu^3\\
&+\mu^2+\tfrac{4}{3}\mu)+\tfrac{3}{2}\mu^2(36\mu^4+30\mu^3-26\mu^2-33\mu-7)\\
=\;& 288\mu^6+207\mu^5-8\mu^4-\tfrac{199}{6}\mu^3-\tfrac{1165}{2}\mu^2+\tfrac{632}{3}\mu-12.
\end{aligned}
$$

- By adding the values of $w^*SZ_v(\mathbb{CNT})$ and $w^*Sz_e(\mathbb{CNT})$, we get

$$w^*Sz_t(\mathbb{CNT})=948\mu^6+\tfrac{7051}{15}\mu^5-\tfrac{4456}{3}\mu^4+\tfrac{1591}{3}\mu^3-\tfrac{799}{6}\mu^2+\tfrac{1261}{10}\mu-44.$$

Theorem 2.7 *For $\mu\geq 2$, the weighted plus Mostar indices of hexagonal boron nitride are*

- $w^+Mo_v(\mathbb{CNT})=48\mu^4+\frac{668}{3}\mu^3-350\mu^2+\frac{340}{3}\mu-16-4\left\lfloor\frac{\mu}{2}\right\rfloor(2(12\mu^2+8\mu+1)\left\lfloor\frac{\mu}{2}\right\rfloor-24\mu^3-16\mu^2+8\mu+1)$.
- $w^+Mo_e(\mathbb{CNT})=72\mu^4+24\mu^3-56\mu^2-60\mu+14+4(6\mu+1)\left\lfloor\frac{\mu}{2}\right\rfloor(6\mu^2+\mu-2-(6\mu+1)\left\lfloor\frac{\mu}{2}\right\rfloor)$.
- $w^+Mo_t(\mathbb{CNT})=96\mu^4+\frac{1336}{3}\mu^3-700\mu^2+\frac{680}{3}\mu-32-4\left\lfloor\frac{\mu}{2}\right\rfloor((60\mu^2+28\mu+3)\left\lfloor\frac{\mu}{2}\right\rfloor-60\mu^3-28\mu^2+19\mu+3)$.

Proof.

- Now, using the equations (6), we have

$$
\begin{aligned}
w^{+}Mo_{v}(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2+3)+2(3+3)(\alpha-1))|4\mu^2+4\mu-1-\alpha(2\alpha+1)-\alpha(2\alpha+1)| \\
& +[2(2+2)+2(3+3)(\mu-1)+2(2+3)+2(3+3)(\mu-1)]|4\mu^2+4\mu-1 \\
& -\mu(2\mu+1)-\mu(2\mu+1)|+2\sum_{\alpha=1}^{\mu-2}(2(2+3)+(3+3)(2\alpha-1))|4\mu^2+4\mu-1 \\
& -\alpha(2\alpha+3)-\alpha(2\alpha+3)|+[2(2+3)+(3+3)(2(\mu-1)-1)+2(2+2) \\
& +(3+3)(2(\mu-1)-1)]|4\mu^2+4\mu-1-(\mu-1)(2(\mu-1)+3)-(\mu-1)(2 \\
& (\mu-1)+3)|+\sum_{\alpha=1}^{\mu}(2(2+2)+(3+3)(\mu-1))|4\mu^2+4\mu-1-(2\mu+1) \\
& (2\alpha-1)-(2\mu+1)(2\alpha-1)|+\sum_{\alpha=1}^{\mu}\mu(3+3)|4\mu^2+4\mu-1-2\alpha(2\mu+1) \\
& -2\alpha(2\mu+1)| \\
= \; & 4\sum_{\alpha=1}^{\mu-1}(6\alpha-1)(4\mu^2+4\mu-1-2\alpha(2\alpha+1))+6(4\mu-1)(2\mu-1) \\
& +8\sum_{\alpha=1}^{\mu-2}(3\alpha+1)(4\mu^2+4\mu-1-2\alpha(2\alpha+3))+6(4\mu-3)(6\mu+1) \\
& +2(3\mu+1)\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}(4\mu^2+4\mu-1-2(2\mu+1)(2\alpha-1))+2(3\mu+1) \\
& \sum_{\alpha=\left\lceil\frac{\mu}{2}\right\rceil+1}^{\mu}(2(2\mu+1)(2\alpha-1)-4\mu^2-4\mu+1)+6\mu\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}(4\mu^2+4\mu \\
& -1-4\alpha(2\mu+1))+6\mu\sum_{\alpha=\left\lceil\frac{\mu}{2}\right\rceil+1}^{\mu}(4\alpha(2\mu+1)-4\mu^2-4\mu+1) \\
= \; & 24\mu^4+\frac{640}{3}\mu^3-400\mu^2+\frac{572}{3}\mu-28+6(4\mu-1)(2\mu-1)+24\mu^4+\frac{64}{3}\mu^3 \\
& -164\mu^2+\frac{116}{3}\mu+24+6(4\mu-3)(6\mu+1)+4\left\lceil\frac{\mu}{2}\right\rceil(3\mu+1)(-2(2\mu+1) \\
& \left\lceil\frac{\mu}{2}\right\rceil+4\mu(\mu+1)-1)-4(3\mu+1)(2\mu^2-\mu)+12\left\lceil\frac{\mu}{2}\right\rceil\mu(-2(2\mu+1)\left\lceil\frac{\mu}{2}\right\rceil \\
& +4\mu^2-3)+6\mu^2(2\mu+3) \\
& =48\mu^4+\frac{668}{3}\mu^3-350\mu^2+\frac{340}{3}\mu-16-4\left\lceil\frac{\mu}{2}\right\rceil(2(12\mu^2+8\mu+1)\left\lceil\frac{\mu}{2}\right\rceil \\
& -24\mu^3-16\mu^2+8\mu+1).
\end{aligned}
$$

- Now, using the equations (6), we have

$$\begin{aligned}
w^{+}Mo_{e}(\mathbb{CNT}) = \; & 2\sum_{\alpha=1}^{\mu-1}(2(2+3)+2(3+3)(\alpha-1))|6\mu^{2}+3\mu-2-\alpha(3\alpha+1)-\alpha(3\alpha-1)| \\
& +[2(2+2)+2(3+3)(\mu-1)+2(2+3)+2(3+3)(\mu-1)]|6\mu^{2}+3\mu-2 \\
& -\mu(3\mu+1)-\mu(3\mu-1)|+2\sum_{\alpha=1}^{\mu-2}(2(2+3)+(3+3)(2\alpha-1))|6\mu^{2}+3\mu-2 \\
& -\alpha(3\alpha+4)-(3\alpha^{2}+2\alpha-1)|+[2(2+3)+(3+3)(2(\mu-1)-1)+2(2+2) \\
& +(3+3)(2(\mu-1)-1)]|6\mu^{2}+3\mu-2-(\mu-1)(3(\mu-1)+4)-(3(\mu-1)^{2} \\
& +2(\mu-1)-1)|+\sum_{\alpha=1}^{\mu}(2(2+2)+(3+3)(\mu-1))|6\mu^{2}+6\mu-2 \\
& -(6\mu+1)\alpha-((6\mu+1)\alpha-(4\mu+1))|+\sum_{\alpha=1}^{\mu}\mu(3+3)|6\mu^{2}+3\mu \\
& -2-(6\mu+1)\alpha-((6\mu+1)\alpha-\mu)| \\
= \; & 4\sum_{\alpha=1}^{\mu-1}(6\alpha-1)(6\mu^{2}+3\mu-2-2\alpha(3\alpha+1))+6(4\mu-1)(\mu-2)+8\sum_{\alpha=1}^{\mu-2}(3\alpha \\
& +1)(6\mu^{2}+3\mu-1-6\alpha^{2}-6\alpha)+6(4\mu-3)(9\mu-1)+2(3\mu+1)\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil} \\
& (6\mu^{2}+10\mu-1-2(6\mu+1)\alpha)+2(3\mu+1)\sum_{\alpha=\left\lceil\frac{\mu}{2}\right\rceil+1}^{\mu}(-6\mu^{2}-10\mu \\
& +1+2(6\mu+1)\alpha)+6\mu\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}(6\mu^{2}+4\mu-2-2(6\mu+1)\alpha) \\
& +6\mu\sum_{\alpha=\left\lceil\frac{\mu}{2}\right\rceil+1}^{\mu}(-6\mu^{2}-4\mu=2+2(6\mu+1)\alpha) \\
= \; & 36\mu^{4}+4\mu^{3}-68\mu^{2}+36\mu-8+240\mu^{2}-240\mu+30+36\mu^{4}+20\mu^{3}-252\mu^{2} \\
& +140\mu-8+2(3\mu+1)[-2(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil^{2}+4(\mu+1)(3\mu-1) \\
& \left\lceil\frac{\mu}{2}\right\rceil+(2-3\mu)\mu]+6\mu[2(6\mu^{2}-2\mu-3)\left\lceil\frac{\mu}{2}\right\rceil-2(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil^{2}+3\mu(\mu+1)] \\
= \; & 72\mu^{4}+24\mu^{3}-56\mu^{2}-60\mu+14+4(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil(6\mu^{2}+\mu-2-(6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil).
\end{aligned}$$

- By adding the values of $w^{+}Mo_{v}(\mathbb{CNT})$ and $w^{+}Mo_{e}(\mathbb{CNT})$, we get

$$\begin{aligned}
w^{+}Mo_{t}(\mathbb{CNT}) = \; & 96\mu^{4}+\tfrac{1336}{3}\mu^{3}-700\mu^{2}+\tfrac{680}{3}\mu-32-4\left\lceil\frac{\mu}{2}\right\rceil((60\mu^{2}+28\mu+3)\left\lceil\frac{\mu}{2}\right\rceil \\
& -60\mu^{3}-28\mu^{2}+19\mu+3).
\end{aligned}$$

Theorem 2.8 *For $\mu \geq 2$, the weighted multiply Mostar indices of hexagonal boron nitride are*

- $w^{*}Mo_{v}(\mathbb{CNT}) = 72\mu^{4}+32\mu^{3}-16\mu^{2}-65\mu+6-2\left\lceil\frac{\mu}{2}\right\rceil((72\mu^{2}+32\mu-2)\left\lceil\frac{\mu}{2}\right\rceil-72\mu^{3}-32\mu^{2}+40\mu-1)$.
- $w^{*}Mo_{e}(\mathbb{CNT}) = 1944\mu^{6}-4752\mu^{5}+1782\mu^{4}+15\mu^{3}-105\mu^{2}+18\mu-14-2\left\lceil\frac{\mu}{2}\right\rceil((108\mu^{2}+12\mu-1)\left\lceil\frac{\mu}{2}\right\rceil-108\mu^{3}-12\mu^{2}+49\mu-2)$.
- $w^{*}Mo_{t}(\mathbb{CNT}) = 1944\mu^{6}-4752\mu^{5}+1854\mu^{4}+47\mu^{3}-121\mu^{2}-65\mu+6-2\left\lceil\frac{\mu}{2}\right\rceil((-180\mu^{2}-44\mu+3)\left\lceil\frac{\mu}{2}\right\rceil+180\mu^{3}+44\mu^{2}-89\mu+3)$.

Proof.

- Now, using the equations (6), we have

$$
\begin{aligned}
w^*Mo_v(\mathbb{CNT}) = {} & 2\sum_{\alpha=1}^{\mu-1}(2(2\times3)+2(3\times3)(\alpha-1))|4\mu^2+4\mu-1-\alpha(2\alpha+1)-\alpha(2\alpha+1)| \\
& +[2(2\times2)+2(3\times3)(\mu-1)+2(2\times3)+2(3\times3)(\mu-1)]|4\mu^2+4\mu-1 \\
& -\mu(2\mu+1)-\mu(2\mu+1)|+2\sum_{\alpha=1}^{\mu-2}(2(2\times3)+(3\times3)(2\alpha-1))|4\mu^2+4\mu-1 \\
& -\alpha(2\alpha+3)-\alpha(2\alpha+3)|+[2(2\times3)+(3\times3)(2(\mu-1)-1)+2(2\times2) \\
& +(3\times3)(2(\mu-1)-1)]|4\mu^2+4\mu-1-(\mu-1)(2(\mu-1)+3)-(\mu-1) \\
& (2(\mu-1)+3)|+\sum_{\alpha=1}^{\mu}(2(2\times2)+(3\times3)(\mu-1))|4\mu^2+4\mu-1-(2\mu+1) \\
& (2\alpha-1)-(2\mu+1)(2\alpha-1)|+\sum_{\alpha=1}^{\mu}\mu(3\times3)|4\mu^2+4\mu-1-2\alpha(2\mu \\
& +1)-2\alpha(2\mu+1)| \\
= {} & 12\sum_{\alpha=1}^{\mu-1}(3\alpha-1)(4\mu^2+4\mu-1-2\alpha(2\alpha+1))+4(9\mu-4)(2\mu-1) \\
& +6\sum_{\alpha=1}^{\mu-2}(6\alpha+1)(4\mu^2+4\mu-1-2\alpha(2\alpha+3))+2(18\mu-17)(6\mu+1) \\
& +(9\mu-1)\sum_{\alpha=1}^{\left\lfloor\frac{\mu}{2}\right\rfloor}(4\mu^2+4\mu-1-2(2\mu+1)(2\alpha-1)) \\
& +(9\mu-1)\sum_{\alpha=\left\lfloor\frac{\mu}{2}\right\rfloor+1}^{\mu}(2(2\mu+1)(2\alpha-1)-4\mu^2-4\mu+1)+9\mu\sum_{\alpha=1}^{\left\lfloor\frac{\mu}{2}\right\rfloor}(4\mu^2+4\mu \\
& -1-4\alpha(2\mu+1))+9\mu\sum_{\alpha=\left\lfloor\frac{\mu}{2}\right\rfloor+1}^{\mu}(4\alpha(2\mu+1)-4\mu^2-4\mu+1) \\
= {} & 36\mu^4+16\mu^3-102\mu^2+62\mu-12+4(9\mu-4)(2\mu-1)+36\mu^4+16\mu^3-240\mu^2 \\
& +110\mu+36+2(18\mu-17)(6\mu+1)+2\left\lfloor\frac{\mu}{2}\right\rfloor(9\mu-1)(-2(2\mu+1)\left\lfloor\frac{\mu}{2}\right\rfloor+4\mu(\mu+1)-1) \\
& -(9\mu-1)(2\mu^2-\mu)+18\mu\left\lfloor\frac{\mu}{2}\right\rfloor(-2(2\mu+1)\left\lfloor\frac{\mu}{2}\right\rfloor+4\mu^2-3)+9\mu^2(2\mu+3) \\
= {} & 72\mu^4+32\mu^3-16\mu^2-65\mu+6-2\left\lfloor\frac{\mu}{2}\right\rfloor((72\mu^2+32\mu-2)\left\lfloor\frac{\mu}{2}\right\rfloor-72\mu^3-32\mu^2+40\mu-1).
\end{aligned}
$$

- Now, using the equations (1), we have

$$
\begin{aligned}
w^*Mo_e(\mathbb{CNT}) = {} & 2\sum_{\alpha=1}^{\mu-1}(2(2\times3)+2(3\times3)(\alpha-1))|6\mu^2+3\mu-2-\alpha(3\alpha+1)-\alpha(3\alpha-1)| \\
& +[2(2\times2)+2(3\times3)(\mu-1)+2(2\times3)+2(3\times3)(\mu-1)]|6\mu^2+3\mu-2 \\
& -\mu(3\mu+1)-\mu(3\mu-1)|+2\sum_{\alpha=1}^{\mu-2}(2(2\times3)+(3\times3)(2\alpha-1))|6\mu^2+3\mu-2 \\
& -\alpha(3\alpha+4)-(3\alpha^2+2\alpha-1)|+[2(2\times3)+(3\times3)(2(\mu-1)-1) \\
& +2(2\times2)+(3\times3)(2(\mu-1)-1)]|6\mu^2+3\mu-2-(\mu-1)(3(\mu-1)+4) \\
& -(3(\mu-1)^2+2(\mu-1)-1)|+\sum_{\alpha=1}^{\mu}(2(2\times2)+(3\times3)(\mu-1))|6\mu^2 \\
& +6\mu-2-(6\mu+1)\alpha-((6\mu+1)\alpha-(4\mu+1))|+\sum_{\alpha=1}^{\mu}\mu(3\times3) \\
& |6\mu^2+3\mu-2-(6\mu+1)\alpha-((6\mu+1)\alpha-\mu)| \\
= {} & 12\sum_{\alpha=1}^{\mu-1}(3\alpha-1)(6\mu^2+3\mu-2-2\alpha(3\alpha+1))+4(9\mu-4)(\mu-2) \\
& +6\sum_{\alpha=1}^{\mu-2}(6\alpha+1)(6\mu^2+3\mu-1-6\alpha^2-6\alpha)+2(18\mu-17)(9\mu-1)
\end{aligned}
$$

$$+(9\mu-1)\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}(6\mu^2+10\mu-1-2(6\mu+1)\alpha)+(9\mu-1)\sum_{\alpha=\left\lfloor\frac{\mu}{2}\right\rfloor+1}^{\mu}(-6\mu^2-10\mu+1$$

$$+2(6\mu+1)\alpha)+9\mu\sum_{\alpha=1}^{\left\lceil\frac{\mu}{2}\right\rceil}(6\mu^2+4\mu-2-2(6\mu+1)\alpha)+9\mu\sum_{\alpha=\left\lfloor\frac{\mu}{2}\right\rfloor+1}^{\mu}(-6\mu^2$$

$$-4\mu+2+2(6\mu+1)\alpha)$$

$$= 54\mu^4-18\mu^3-96\mu^2+84\mu-24+4(9\mu-4)(\mu-2)54\mu^4+6\mu^3-360\mu^2+276\mu-24$$

$$+2(18\mu-17)(9\mu-1)-2(9\mu-1)\left\lceil\frac{\mu}{2}\right\rceil((6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil-6\mu^2-4\mu+2)$$

$$+27\mu^2(\mu+1)-18\mu\left\lceil\frac{\mu}{2}\right\rceil((6\mu+1)\left\lceil\frac{\mu}{2}\right\rceil-6\mu^2+2\mu+3)$$

$$= 1944\mu^6-4752\mu^5+1782\mu^4+15\mu^3-105\mu^2+18\mu-14-2\left\lceil\frac{\mu}{2}\right\rceil((108\mu^2+12\mu$$

$$-1)\left\lceil\frac{\mu}{2}\right\rceil-108\mu^3-12\mu^2+49\mu-2).$$

- By adding the values of $w^*Mo_v(\mathbb{CNT})$ and $w^*Mo_e(\mathbb{CNT})$, we get

$$w^*Mo_t(\mathbb{CNT}) = 1944\mu^6-4752\mu^5+1854\mu^4+47\mu^3-121\mu^2-65\mu+6-2\left\lceil\frac{\mu}{2}\right\rceil((-180\mu^2-44\mu$$

$$+3)\left\lceil\frac{\mu}{2}\right\rceil+180\mu^3+44\mu^2-89\mu+3).$$

Numerical and graphical Comparison of results for the Hexagonal Boron nitride and Carbon nanotube

The Mostar, PI, and Szeged type indices for hexagonal boron nitride and carbon nanotube structures are thoroughly compared numerically and graphically in this section. According to the analytical results presented in Sections 2, the Szeged indices have a hexic (sixth-degree polynomial) growth trend, while the Mostar and PI indices show a quadratic growth pattern with respect to the parameter μ. Tables 1, 2, and 3 summarize the results of our computation of the indices for values of μ (ranging from 2 to 10) in order to support these observations. The Mostar, PI, and Szeged indices based on vertex distance are reported in Table 1, and their counterparts based on edge distance are given in Table 2. Table 3 displays the indices based on total distance. A thorough quantitative comparison between various formulations is made possible by the inclusion of both the classical forms of the indices and their weighted variants (w^+ and w^* in each table).

Figure 2 show how these indices behave graphically. The variation of the vertex-distance based indices is shown in Figure 2, the corresponding trends for the edge-distance based indices are shown in Figure 2, and the total-distance based indices are shown in Figure 2. These numbers unmistakably show how quickly the indices, especially the Szeged-type measures, have increased, supporting their higher-order growth. The visual comparison offers more insight into the structural properties of the carbon nanotube by highlighting the distinctions between the weighted and un-weighted versions.

$[\mu]$	Mo_v	Sz_v	w^+PI_v	w^+Sz_v	w^+Mo_v	w^*PI_v	w^*Sz_v	w^*Mo_v
2	270	2830	3312	13680	1796	4370	33125	1770
3	1237	24516	15510	127168	8954	20915	444374	8879
4	3890	117652	46452	635188	28248	63832	2637426	29590
5	9025	405122	109242	2240884	65390	152201	10292466	70643
6	18478	1125810	220440	6326888	132268	310286	31061295	147978
7	33285	2691752	400062	15295160	236034	567535	78737298	270495

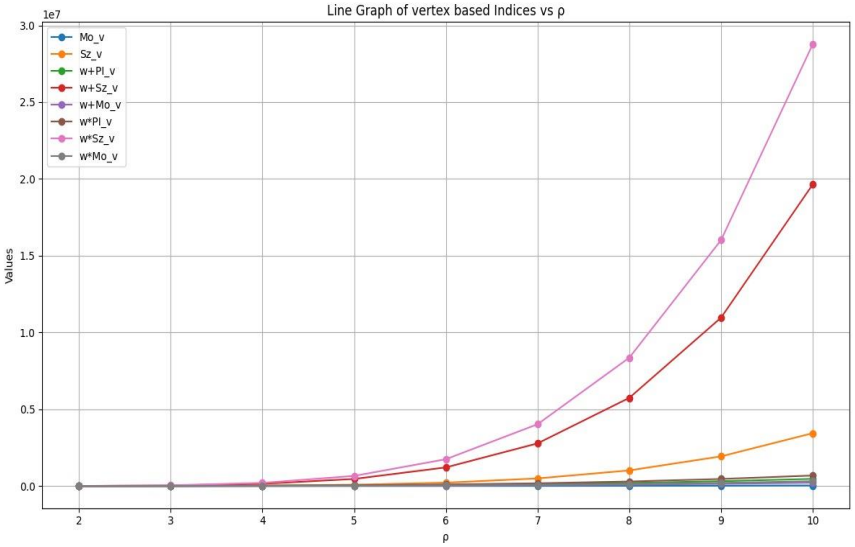
8	56258	5756808	671580	32975948	394432	958580	175900612	462918
9	88545	11296854	1061922	65105868	615286	1523237	357038494	735155
10	134062	20701494	1601472	119875104	922964	2306506	672140889	1121866

Table 1: Vertex-distance based Mostar, PI and Szeged indices of Carbon nanotube

$[\mu]$	Mo_e	Sz_e	w^+PI_e	w^+Sz_e	w^+Mo_e	w^*PI_e	w^*Sz_e	w^*Mo_e
2	352	2902	4320	14198	1586	5320	22742	1308
3	1693	32381	20778	159954	8394	27145	254087	409742
4	5410	176468	63480	873252	28446	85648	1378956	3565546
5	12757	656486	151434	3251652	68634	208477	5124208	16669756
6	26312	1922126	308832	9527770	144530	431056	15009310	56126284
7	47785	4772407	565050	23672206	265330	796585	37304297	153247814
8	81106	10502556	954648	52126072	455246	1356040	82195092	361415730
9	128281	21076808	1517370	104663120	724626	2168173	165156186	764564636
10	194752	39327126	2298144	195381470	1107474	3299512	308530678	1487165836

Table 2: Edge-distance based Mostar, PI and Szeged indices of Carbon nanotube

$[\mu]$	Mo_t	Sz_t	w^+PI_t	w^+Sz_t	w^+Mo_t	w^*PI_t	w^*Sz_t	w^*Mo_t
2	668	4619	7632	27878	3728	9690	55867	512
3	3214	46657	36288	287122	18612	48060	698461	406629
4	10256	243306	109932	1508440	59224	149480	4016382	3548958
5	24182	882677	260676	5492536	137344	360678	15416674	16632239
6	49840	2542545	529272	15854658	279032	741342	46070605	56037648
7	90506	6240685	965112	38967366	498660	1364120	116041595	153089781
8	153548	13616888	1626228	85102020	835632	2314620	258095704	361129862
9	242842	27146657	2579292	169768988	1304992	3691410	522194680	764117223
10	368564	50386583	3899616	315256574	1961408	5606018	980671567	1486460976



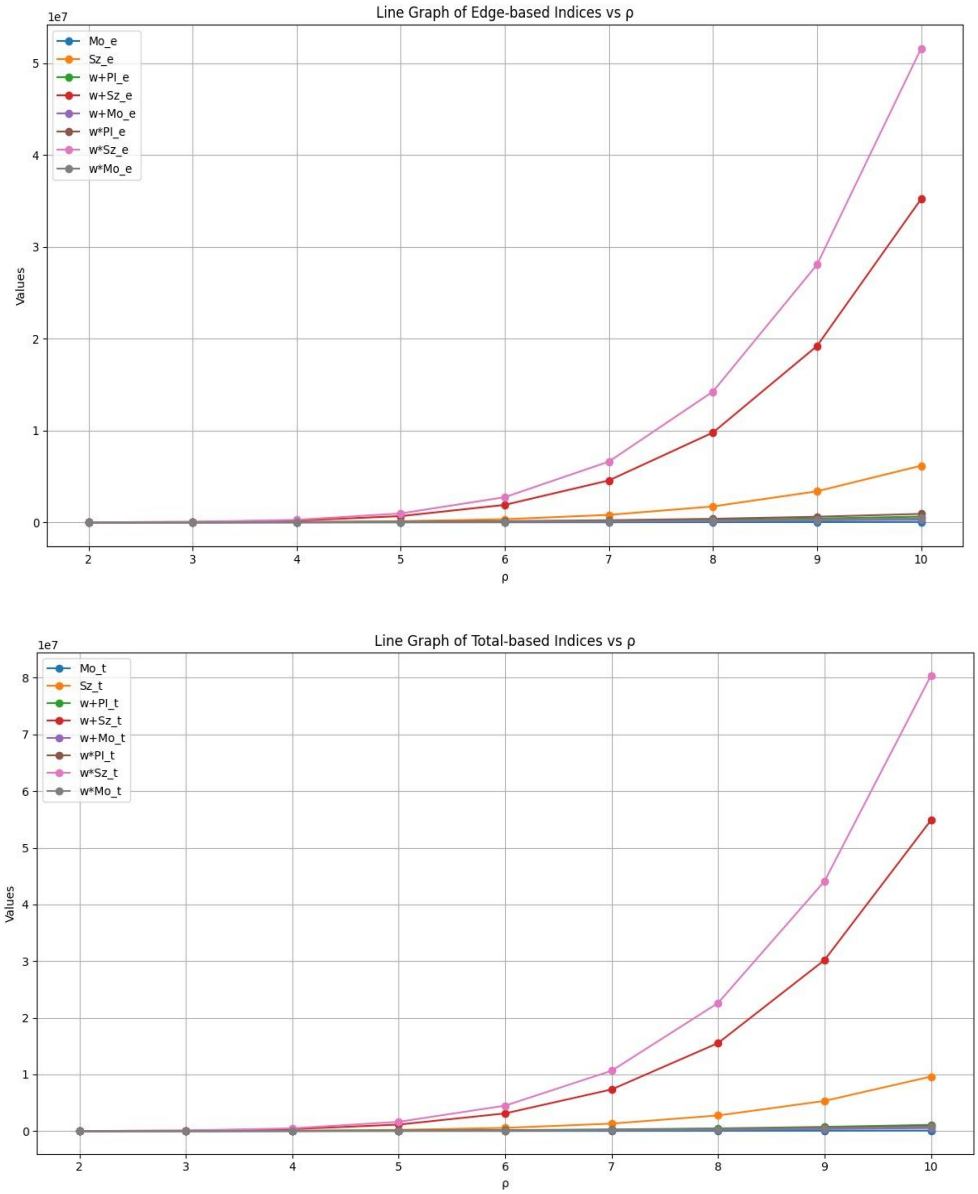


Figure 2: Comparison of Vertex-distance based, edge-distance based and total-distance based Mostar, PI and Szeged indices of Carbon nanotube

Conclusion

The Mostar, Padmakar-Ivan (PI), and Szeged type indices for the molecular graphs of carbon nanotubes and hexagonal boron nitride nanotubes have been studied in this work. We were able to derive exact closed-form expressions for vertex-distance, edge-distance, and total-distance based indices, as well as their weighted variants, by using the cut method. Different growth patterns of these indices are revealed by the numerical results and graphical analysis. Specifically, the Mostar and PI indices show quadratic behavior, while the Szeged indices show a hexic trend and much faster growth. These findings are backed up by tabulated data and graphical representations that make it easy to

compare various index types. The acquired findings advance our theoretical knowledge of topological descriptors and how they behave on intricate nanostructures. Additionally, the study emphasizes how well the cut method works for large and regular graph structures when calculating distance-based indices. These results are anticipated to be helpful in future research on chemical graph theory, nanotechnology, and the creation of QSAR/QSPR models.

REFERENCES

[1] M. O. Albertson, The irregularity of a graph, Ars Comb., 46, 1997, 219–225.
[2] M. Arockiaraj, J. Clement, N. Tratnik, Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems, Int. J. Quantum Chem., 119(24), 2019, e26043.
[3] S. Akhter, M. Imran, Z. Iqbal, Mostar indices of SiO_2 nanostructures and melem chain nanostructures, Int. J. Quantum Chem., 2020, e26520.
[4] S. Akhter, Z. Iqbal, A. Aslam, W. Gao, Computation of Mostar index for some graph operations, International Journal of Quantum Chemistry, 121(15), 2021, e26674.
[5] M. M. Dehmer, N. N. Barbarini, K. K. Varmuza, A. A. Graber, Novel topological descriptors for analyzing biological networks, BMC Struc. Biol., 10(1), 2010, 18.
[6] T. Došlić, I. Martinjak, R. Škrekovski, S. T. Spužević, I. Zubac, Mostar index, J. Math. Chem., 56(10), 2018, 2995–3013.
[7] K. Deng, S. Li, Extremal catacondensed benzenoids with respect to the Mostar index, J. Math. Chem., 58(7), 2020, 1437–1465.
[8] M. R. Farahani, M. K. Jamil, M. Imran, Vertex PI_v topological index of titania carbon nanotubes $TiO_2(m,n)$, Appl. Math. and Nonli. Sci., 1(1), 2016, 175–182.
[9] M. R. Farahani, Computing Edge-PI index and Vertex PI index of circumcoronene series of benzenoid H_k by use of cut method, Int. J. Math. Model. and Appl. Comput., 1(6), 2013, 41–50.
[10] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17(4), 1972, 535–538.
[11] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, Graph Theory Notes New York, 27(9), 1994, 9–15.
[12] I. Gutman, Degree-based topological indices , Croatica Chemica Acta, 86(4), (2013) 351–361.
[13] W. Gao, W. Wang, M. R. Farahani, Topological indices study of molecular structure in anticancer drugs, J. Chem., 2016(1), 2016, 3216327.
[14] W. Gao, M. R. Farahani, L. Shi, The forgotten topological index of some drug structures, Acta Medica Mediterranea, 32(1), 2016, 579–585.
[15] W. Gao, S. Akhter, Z. Iqbal, M. Qasim, A. Aslam, The topological aspects of Phthalocyanines and Porphyrins dendrimers, IEEE Access, 8, 2020, 168631–168649.
[16] M. Imran, S. Akhter, Z. Iqbal, Edge Mostar index of chemical structures and nanostructures using graph operations, Int. J. Quantum Chem., 120(15), 2020, e26259.
[17] S. Klavžar, I. Gutman, B. Mohar, Labeling of benzenoid systems which reflects the vertex-distance relations, J. Chem. Inf. Model., 35(3), 1995, 590–593.
[18] S. Klav ž ar, On the canonical metric representation, average distance, and partial Hamming graphs, Eur. J. Combinatorics, 27(1), 2006, 68–73.
[19] S. Klav ž ar, S. Li, H. Zhang, On the difference between the (revised) Szeged index and the Wiener index of cacti, Discrete Appl. Math., 247, 2018, 77–89.

[20] S. Kang, Z. Iqbal, M. Ishaq, R. Sarfraz, A. Aslam, W. Nazeer, On eccentricity-based topological indices and polynomials of phosphorus-containing dendrimers, Symmetry, 10(7), 2018, 237.
[21] S. M. Kang, M. A. Zahid, W. Nazeer, W. Gao, Calculating the degree-based topological indices of dendrimers, Chemistry, 16(1), 2018, 681–688.
[22] S. M. Kang, W. Nazeer, M. A. Zahid, A. R. Nizami, A. Aslam, M. Munir, M-polynomials and topological indices of hexderived networks, Physics, 16(1), 2018, 394-403.
[23] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, J. Chem. Inf. Comput. Sci., 41(4), 2001, 934–949.
[24] S. Li, H. Zhang, Proofs of three conjectures on the quotients of the (revised) Szeged index and the Wiener index and beyond, Discrete Math., 340(3), 2017, 311–324.
[25] T. Pisanski, M. Randić, Use of the Szeged index and the revised Szeged index for measuring network bipartivity, Discrete Appl. Math., 158(17), 2010, 1936–1944.
[26] R. V. Solé, S. Valverde, Information theory of complex networks: on evolution and architectural constraints, In compl. Sprin. Berl. Heid, 2014, 189–207.
[27] N. Tratnik, Computing the Mostar index in networks with applications to molecular graphs, 2019, arXiv:1904.04131.
[28] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc., 69(1), 1947, 17–20.
[29] J. Zheng, M. R. Farahani, M. K. Jamil, M. K. Siddiqui, X. Zhang, The edge-Padmakar-Ivan index of the Iitania nanotubes, Int. J. of Pharm. Scien. and Res., 9(3), 2018, 1274–1280.

IEER
Institute for Excellence in Education & Research